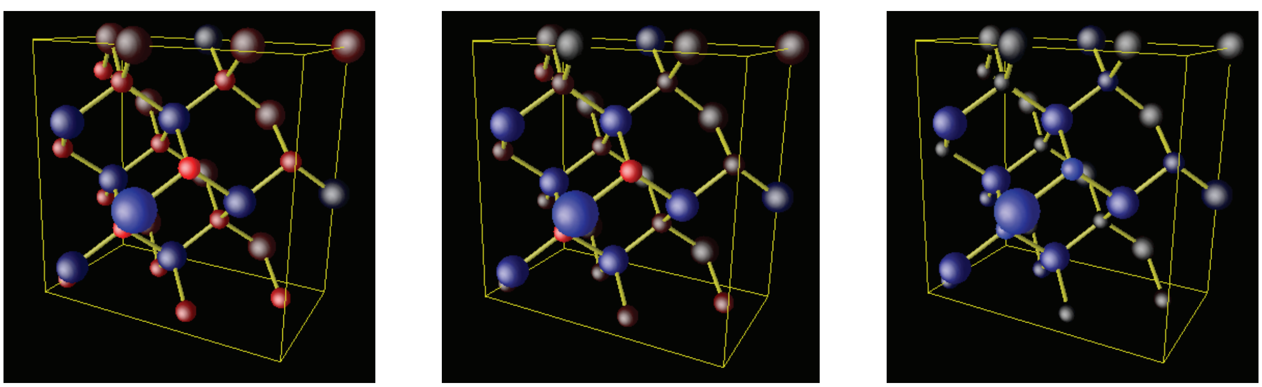
New Insight into Semiconductors Appears in *Nature Materials*

Results of investigations of the electronic and magnetic properties of semiconductors by researchers from Oak Ridge National Laboratory, Daresbury Laboratory, and the University of Alabama appear in an upcoming issue of *Nature Materials* (Advanced Online Publication, 23 October 2005 | doi:10.1038/nmat1509). The team employed resources of the National Center for Computational Sciences (NCCS), located at Oak Ridge National Laboratory, to carry out their novel analysis of the nature of electronic structure and magnetic exchange in doped semiconductors.

Traditional semiconductors revolutionized industry and helped define the computer era. Conductivity in these materials may be dramatically altered by ‘doping’ with impurities. Doped polycrystalline silicon is commonly used in integrated circuits.

Magnetic semiconductors possess the fundamental nature of semiconductors with the additional property dimension of ferromagnetism. Future generations of electronic devices may combine these properties: transmitting information by charge and using electronic spin to process, store, or manipulate data.



Mn (large sphere) in GaAs, GaP, and GaN, respectively. The color encodes the magnetization on the particular lattice site. Blue means aligned with the moment of the Mn impurity. Red means anti-aligned.

The *Nature Materials* paper helps resolve long-standing discrepancies between phenomenological models, widely used to describe properties of new semiconductor materials, and first-principles electronic structure descriptions of magnetic semiconductors. Paradoxically, the researchers’ first-principles calculations verified the validity of the phenomenological studies and identified a potential flaw in other ab initio models that are typically—and perhaps incorrectly—applied to research of magnetic semiconductors.

The computational resources of the NCCS enabled the large, accurate calculations needed to replicate from first principles the subtle interactions between electronic and magnetic forces as well as other experimentally measurable properties in doped magnetic semiconductors. Predicting doped semiconductor materials that retain magnetic order at room temperature is the ultimate achievement of this research and opens the door to the development of novel devices.